# Multiple Lifshitz transitions driven by short-range antiferromagnetic correlations in the two-dimensional Kondo lattice model

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**Abstract.** With a mean field approach, the heavy Fermi liquid in the two-dimensional Kondo lattice model is carefully considered in the presence of short-range antiferromagnetic correlations. As the ratio of the local Heisenberg superexchange coupling to the Kondo coupling increases, the Fermi surface structure changes dramatically. From the analysis of the ground state energy density, multiple Lifshitz type phase transitions occur at zero temperature.

### 1. Introduction

Quantum phase transitions have attracted much interest in studying correlated electron systems. An electronic phase transition associated with the change of Fermi surface (FS) topology, the so-called Lifshitz transition[1], can be induced without any spontaneous symmetry breaking and local order parameter. The Kondo lattice model is a prototype model and believed to capture the basic physics of heavy fermion materials. The huge mass enhancement of the quasiparticles can be attributed to the coherent superposition of individual Kondo screening clouds, and the resulting metallic state is characterized by a large FS with the Luttinger volume containing both conduction electrons and localized moments. Competing with the Kondo singlet formation, the localized spins indirectly interact with each other via magnetic polarization of the conduction electrons – the Ruderman-Kittel-Kasuya-Yosida interaction. Such an interaction dominates at low values of the Kondo exchange coupling and is the driving force for the antiferromagnetic (AFM) long-range order and quantum phase transitions [2, 3]. So far most of investigations focus on the possible FS reconstruction around the magnetic quantum critical point [4, 5, 6, 7, 8]. However, the FS topology in the paramagnetic heavy fermi liquid phase may also be drastically changed by the short-range AFM spin correlations between the localized spins, leading to the Lifshitz phase transitions [9]. The nature of such a quantum phase transition has not been thoroughly explored yet.

In this paper, we consider the two-dimensional Kondo lattice model with the Heisenberg AFM superexchange coupling between localized spins. By introducing uniform short-range AFM valence-bond and Kondo screening parameters, a fermionic mean-field theory is derived and carefully re-examined. Away from half-filling, at the conduction electron density  $n_c = 0.85$ , for example, the possible changes of FS topology in the paramagnetic heavy Fermi liquid phase are considered carefully as increasing the short-range AFM spin correlations.

#### 2. Mean field theory

The model Hamiltonian defined on a square lattice is given by

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + J_K \sum_{i} \mathbf{S}_i \cdot \mathbf{s}_i + J_H \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j.$$
 (1)

The spin-1/2 operators of the local magnetic moments have the fermionic representation  $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma\sigma'} f_{i\sigma}^{\dagger} \tau_{\sigma\sigma'} f_{i\sigma'}$  with a local constraint  $\sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} = 1$ , where  $\tau$  is the Pauli matrices. Following the large-N fermionic approach[10], the Kondo spin exchange and Heisenberg superexchange terms can be expressed up to a chemical potential shift as

$$\mathbf{S}_{i} \cdot \mathbf{S}_{j} = -\frac{1}{2} \sum_{\sigma \sigma'} f_{i\sigma}^{\dagger} f_{j\sigma} f_{j\sigma'}^{\dagger} f_{i\sigma'}, \qquad \mathbf{S}_{i} \cdot \mathbf{s}_{j} = -\frac{1}{2} \sum_{\sigma \sigma'} f_{i\sigma}^{\dagger} c_{j\sigma} c_{j\sigma'}^{\dagger} f_{i\sigma'}, \tag{2}$$

then uniform short-range AFM valence bond and Kondo screening order parameters can be introduced as

$$\chi = -\sum_{\sigma} \left\langle f_{i\sigma}^{\dagger} f_{i+l\sigma} \right\rangle, \qquad V = \sum_{\sigma} \left\langle c_{i\sigma}^{\dagger} f_{i\sigma} \right\rangle. \tag{3}$$

To avoid the incidental degeneracy of the conduction electron band on a square lattice, we choose  $\epsilon_{\mathbf{k}} = -2t \left(\cos k_x + \cos k_y\right) + 4t' \cos k_x \cos k_y - \mu$ , where t and t' are the first and second nearest neighbor hoping matrix elements, respectively, while  $\mu$  is the chemical potential, which should be determined self-consistently by the density of the conduction electrons  $n_c$ . Under the uniform mean-field approximation, the f-spinons form a very narrow band with the dispersion  $\chi_{\mathbf{k}} = J_H \chi \left(\cos k_x + \cos k_y\right) + \lambda$ , where  $\lambda$  is the Lagrangian multiplier to be used to impose the local constraint on average.

Thus the corresponding mean-field Hamiltonian reads

$$H = \sum_{\mathbf{k}\sigma} \begin{pmatrix} c_{\mathbf{k}\sigma}^{\dagger} & f_{\mathbf{k}\sigma}^{\dagger} \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & -\frac{1}{2}J_{K}V \\ -\frac{1}{2}J_{K}V & \chi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{pmatrix} + E_{0}, \tag{4}$$

with  $E_0 = N(-\lambda + J_H \chi^2 + J_K V^2/2)$ . The quasiparticle excitation spectra can be easily obtained

$$E_{\mathbf{k}}^{\pm} = \frac{1}{2} \left[ \left( \epsilon_{\mathbf{k}} + \chi_{\mathbf{k}} \right) \pm W_{\mathbf{k}} \right], \tag{5}$$

which implies that the conduction electron band  $\epsilon_{\mathbf{k}}$  has a finite hybridization with the spinon band  $\chi_{\mathbf{k}}$ . Here  $W_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \chi_{\mathbf{k}})^2 + (J_K V)^2}$ . Accordingly, the ground-state energy density can be evaluated as

$$\varepsilon_g = \frac{2}{N} \sum_{\mathbf{k}, +} E_{\mathbf{k}}^{\pm} \theta \left( -E_{\mathbf{k}}^{\pm} \right) - \lambda + J_H \chi^2 + \frac{1}{2} J_K V^2, \tag{6}$$

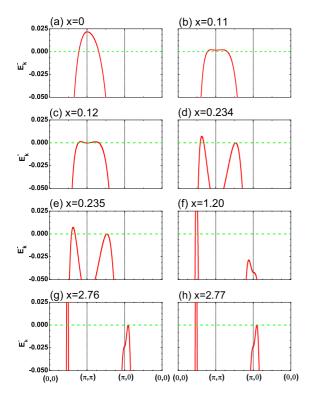
where  $\theta(-E_{\mathbf{k}})$  is the theta function. Then the self-consistent equations for the mean-field variables  $\chi$ , V, and  $\lambda$  and the chemical potential  $\mu$  can be deduced from the relations

$$\frac{\partial \varepsilon_g}{\partial \chi} = 0, \quad \frac{\partial \varepsilon_g}{\partial V} = 0, \quad \frac{\partial \varepsilon_g}{\partial \lambda} = 0, \quad n_c = -\frac{\partial \varepsilon_g}{\partial \mu}.$$
 (7)

## 3. Results and Discussions

In the following, we will assume that t'/t = 0.1 and  $n_c = 0.85$ . When the self-consistent equations are carefully evaluated, we find that the mean-field AFM order parameter  $\chi$  is always positive in the range  $0 < J_H/J_K \le 3$  so that the resulting state is a stable paramagnetic metal.

In Fig.1, as the strength of the AFM spin fluctuations grows up, we present the evolution of the band structure of the renormalized heavy quasiparticles around the Fermi level in the direction  $(0,0) \to (\pi,\pi) \to (\pi,0) \to (0,0)$  of the first Brillouin zone. Fig.1a to Fig.1h correspond to  $J_K/t=2.0$  and  $x=J_H/J_K=0$ , 0.11, 0.12, 0.234, 0.235, 1.2, 2.76, and 2.77, respectively. At the critical values x=0.1181, the point  $(\pi,\pi)$  changes from the local maximum to local minimum of the quasiparticle band, while at x=0.2341, the separated band around the momentum  $(\pi,\pi/2)$  starts to move away from the Fermi level. As the ratio of the coupling strengths increases, the separated band moves to the momentum  $(\pi,0)$ , and reaches the Fermi level again at x=2.77.



**Figure 1.** The lower renormalized quasiparticle band in the direction  $(0,0) \to (\pi,\pi) \to (\pi,0) \to (0,0)$  as increasing the strength of the AFM spin fluctuations.

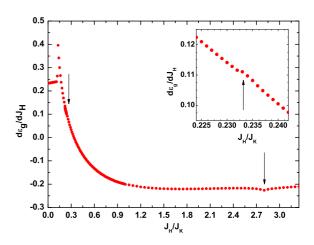
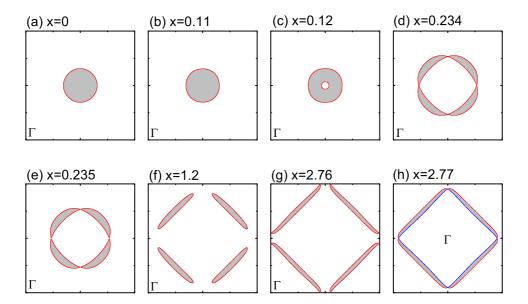


Figure 2. The first-order derivative of the ground state energy as a function of the parameter  $x = J_H/J_K$ . There are three singular points,  $x_{c,1} = 0.1181$ ,  $x_{c,2} = 0.2341$ , and  $x_{c,3} = 2.77$ . The first one corresponds to a first order transition, while the latter two correspond to two second order phase transitions, respectively.

From the quantum phase transition aspects, we calculate the ground state energy density  $\varepsilon_g$  and its first-order derivative with respect to the ratio of the coupling parameters x. The numerical results are displayed in Fig.2. We find that there are three non-analytical points.  $\varepsilon_g$  is finite and continuous in the parameter range 0 < x < 3, However, its first-order derivative has a large jump at  $x_{1c} = 0.1181$ , corresponding to a first-order quantum phase transition. Moreover, two small kinks appear at  $x_{2c} = 0.2341$  and  $x_{3c} = 2.77$  in the first-order derivative, which correspond to the jumps in the second-order derivative of  $\varepsilon_g$ . So  $x_{2c}$  and  $x_{3c}$  denote two second-order quantum phase transitions.

Once the renormalized quasiparticle band structure is available, the corresponding FS can be easily obtained. The obtained FS is the large hole-like one and shown as the shaded area. In Fig.3a-3g, the center of the FS is shifted from (0,0) to  $(\pi,\pi)$ . For a fixed  $J_K/t=2.0$ , we can see that the FS is a hole-like circle around  $(\pi,\pi)$  for the parameter range  $0 \le x \le 0.11$ . At  $x_{1c}=0.1181$ , the topology of the FS starts to change: a small circle emerges in the center



**Figure 3.** The structure of the FS changes as increasing the strength of the AFM spin fluctuations. The shaded area represents the hole-like FS. The center of the FS is shifted at  $(\pi, \pi)$  in (a)-(g).

of the deformed large square FS. As x is further increased, both circles expand and the small one is deformed into a rotated square. Up to  $x_{2c} = 0.2341$ , the two deformed circles intersect each other and then decompose into four Fermi pockets. When x increases to  $x_{3c} = 2.77$ , the FS pockets are reconnected again and form two closed square-like circles. Three critical values correspond to three different quantum phase transitions, which belong to the category of Lifshitz phase transitions.

To some extent our present mean-field theory captures the heavy-fermion liquid physics of the Kondo-Heisenberg lattice systems, especially the Fermi surface evolution of the renormalized heavy quasiparticles as the short-range AFM spin correlations between the localized magnetic moments are gradually increased. In order to put the present results on a more solid ground, further investigation beyond the mean-field theory is certainly needed.

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